To exploit the elasto-mechanical properties of nanotubes, researchers at Ames Research Center and Stanford University have focused on using the nanotube as the tip in scanning-probe microscopes (SPM) to perform nanolithography on semiconductor surfaces. Simulations and experiments have shown that nanotubes are the smallest and strongest nanopencils that can read and write in nanoscale. Nanotube tips have enabled continuous lithography of 10 nanometer features, at a speed of up to 0.5 millimeters per second, over large silicon surface areas while simultaneously minimizing the tip-wear problem in conventional SPM-based nanolithography.

The search for low-cost, lightweight molecular hydrogen fuel storage and carrier material in solid booster rockets is crucial because of the potential it holds for effecting big reductions in overall system weight. Fullerenes, or nanotubes, are excellent candidates for they are lightweight, have large surface-to-volume ratios, and provide good adsorption characteristics for molecular hydrogen. Ames has shown in computer simulations that if nanotubes can be opened or closed in a controlled way, inner cavities of the nanotubes can be accessed for storing molecular hydrogen at higher pressures and densities than possible by any other means. The second figure shows that interstitial spacings in nanotube rope

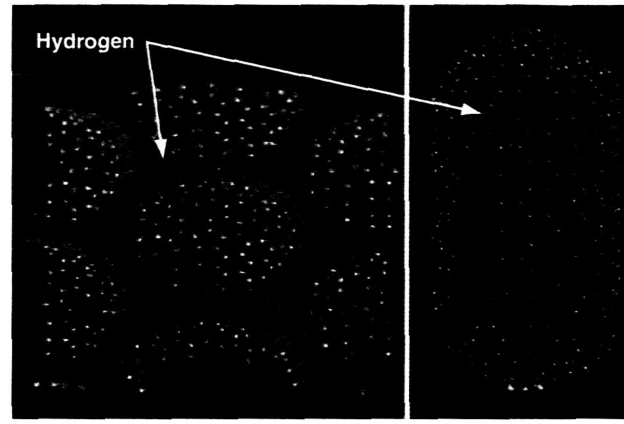

Fig. 2. Hydrogen storage in carbon nanotube: interstitial spacings in a carbon-nanotube rope; red denotes molecular hydrogen.

provide less volume to the stored hydrogen than storage within a closed-end nanotube. Computer simulations in conjunction with experimental efforts investigate the possibility of storing molecular hydrogen in nanotubes as nanoscale gas cylinders that can be carried on future space missions.

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Nanoelectronic Devices for the 21st Century

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Both physical and economic considerations indicate that the scaling era of complementary metal oxide semiconductor will run out of steam around the year 2010. However, physical laws also indicate that it is possible to compute at a rate of a billion times the present speeds with the expenditure of only 1 watt of electrical power. NASA has long-term goals for which ultrasmall semiconductor devices will be needed in critical applications: high-performance, low-power, compact computers for intelligent autonomous vehicles and petaflop (10^{15}) computing technology are two key examples.

Ames Research Center has developed a Green's-function-based code to calculate the transport properties of carbon nanotubes (CNTs). The single most important promise of CNTs with regard to device application is their use as quantum wires. An important question is how disorder affects the conductance of these low-dimensional systems. To obtain an understanding of this, both the low-bias conductance, as a function of the gate voltage (Fermi energy), and the conductance as a function of the applied bias in a CNT for two models of disorders, have been computed. These calculations show that in the presence of weak uniform disorder, the low-bias conductance exhibits a dip as the Fermi energy is swept across the intersection of the first and second sub-bands, as shown in the first figure; otherwise, the CNTs behave as a robust quantum wire. It was also found that in the presence of strong isolated defects, the conductance is significantly affected at the band center, also shown in the first figure.

Silicon-based transistor electronics face daunting technical challenges because of the dramatic miniaturization that is anticipated in the next decade. At that point of miniaturization, identically designed transistors will begin to show different characteristics, a result of uncontrollable deviations in microscopic structure.

A solution to the problem is to greatly simplify the device structure and to build electronics only with atomically precise elements on a regulated surface, as shown in the second figure. This so-called "atomic chain electronics," proposed by Ames as an alternative to silicon-based transistor electronics, will lead to the small and light electronics that will be needed for future NASA space missions. The electronic properties of silicon and magnesium chains have been studied at Ames, with a tight-binding method, and it has been found that silicon chains are always metallic and that magnesium chains are always semiconducting, unlike their three-dimensional counterparts. This indicates that even basic properties have to be reexamined in a microscopic world.

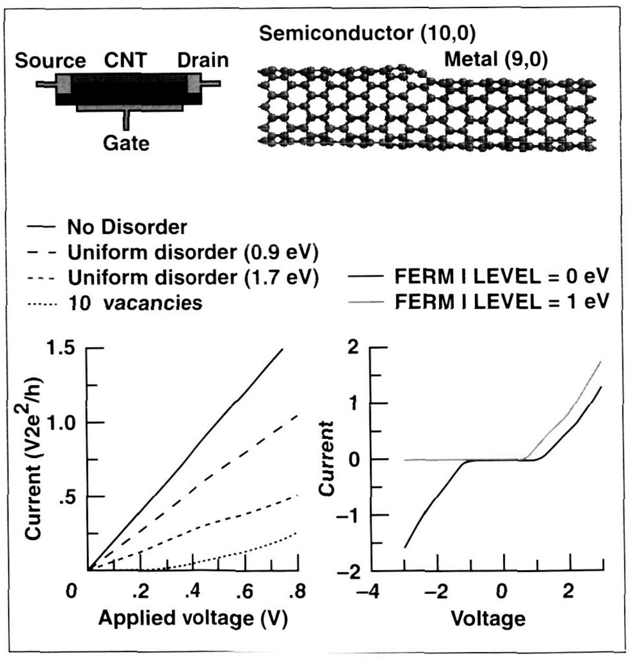

Fig. 1. Comparison of the low-bias conductance versus gate voltage for a defect-free CNT wire and a wire with a weak uniform disorder and strong isolated defects.

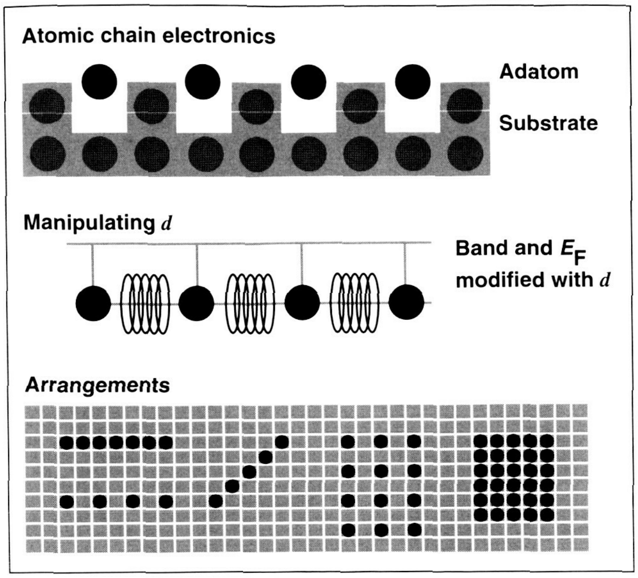

Fig. 2. Device evolution: classic macroscopic (10 years ago), quantum mesoscopic (in next 10 years), and atomic devices (in next 20 years).

Ames is also developing simulation tools that are appropriate for modeling future electronics devices in which both classic and quantum effects are important. The density-gradient model has been incorporated into the partial differential equation solver PROPHET, which was used for quantum-corrected simulations of P-N diodes. A simulation tool called SQUADS, based on the quantum Wigner function and transfer-matrix methods, was used to model devices such as the resonant tunneling diode (RTD), which are quantum-scale in only one dimension. One investigation determined the detailed physics behind strong bistability and 2.5 terahertz oscillations observed in simulations of a particular RTD. These effects were found to be very sensitive to scattering rate and temperature, and it was shown that they could be enhanced with careful modifications of the RTD structure.

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